

chain nodes :
 1 3 4 5 12 15 17 18 19 20

ring nodes :
 6 7 8 9 10 11

chain bonds :
 1-12 3-4 3-12 4-5 5-8 15-17 17-18 18-19 18-20

ring bonds :
 6-7 6-11 7-8 8-9 9-10 10-11

exact/norm bonds :
 1-12 3-12 5-8 18-20

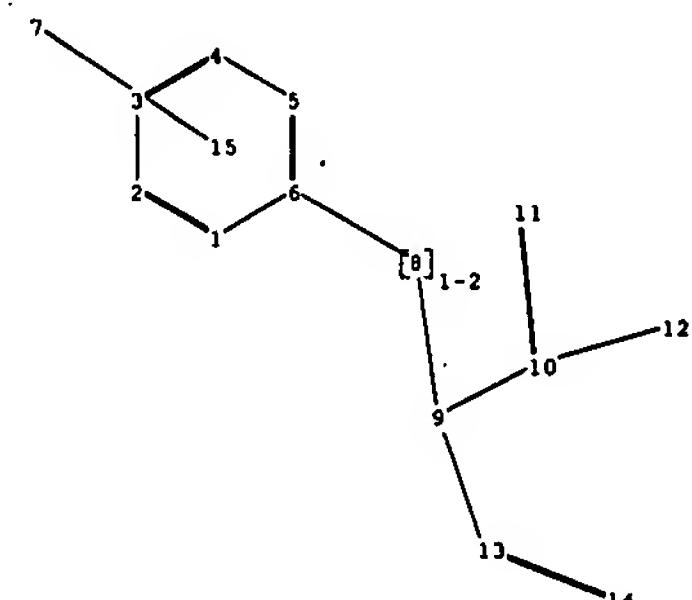
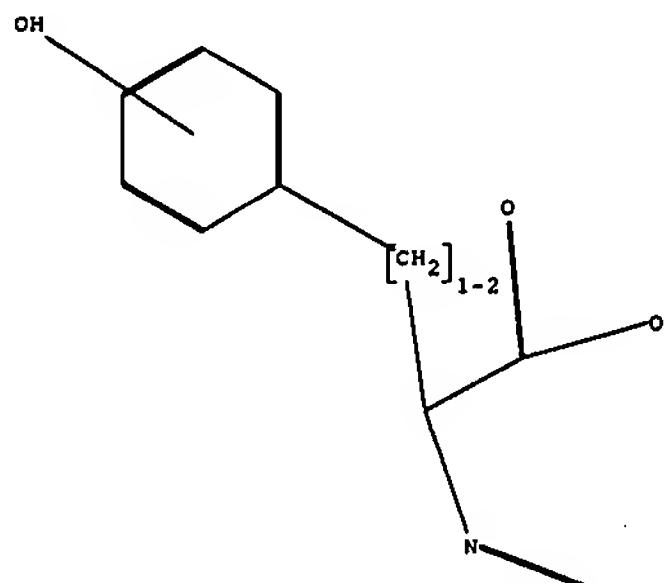
exact bonds :
 3-4 4-5 15-17 17-18 18-19

normalized bonds :
 6-7 6-11 7-8 8-9 9-10 10-11

isolated ring systems :
 containing 6 :

Connectivity :
 1:1 E exact RC ring/chain

Match level :
 1:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
 11:Atom 12:Atom 15:CLASS 16:Atom 17:CLASS 18:CLASS 19:CLASS 20:CLASS



chain nodes :
7 8 9 10 11 12 13 14

ring nodes :
1 2 3 4 5 6

chain bonds :
6-8 8-9 9-10 9-13 10-11 10-12 13-14

ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6

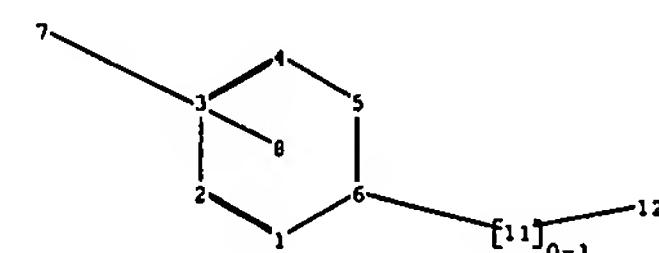
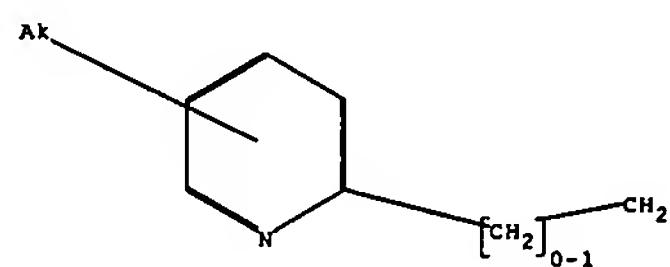
exact/norm bonds :
9-13 10-11 10-12 13-14

exact bonds :
6-8 8-9 9-10

normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:Atom

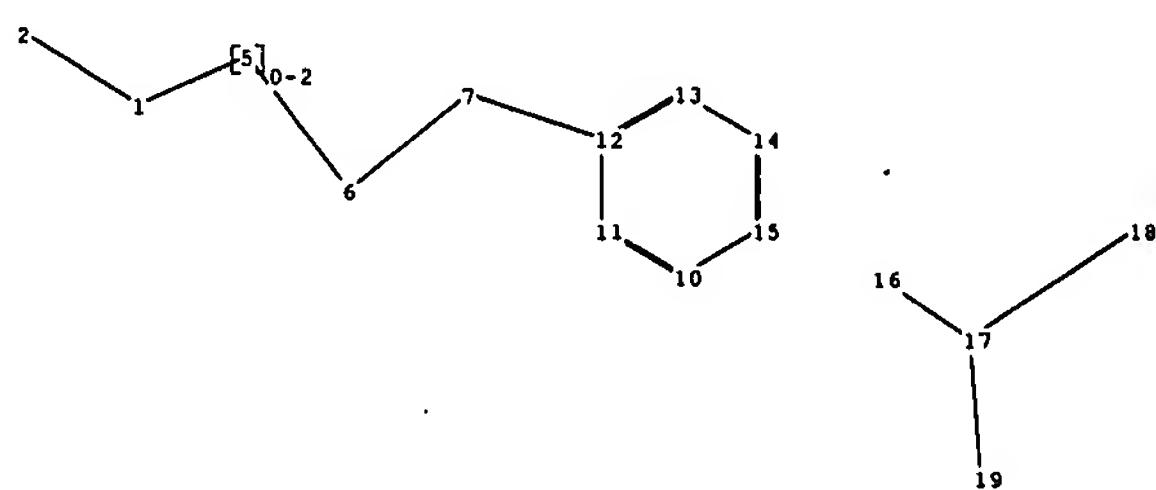
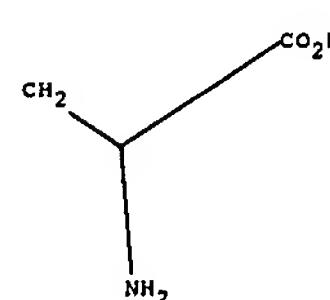
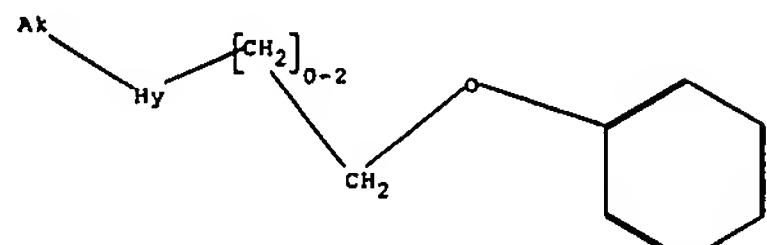


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chain nodes :
 7 11 12
ring nodes :
 1 2 3 4 5 6
chain bonds :
 6-11 11-12
ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
exact bonds :
 6-11 11-12
normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
  containing 1 :

Connectivity :
 7:1 E exact RC ring/chain
Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:Atom 11:CLASS
 12:CLASS

```



chain nodes :

1 2 5 6 7 16 17 18 19

ring nodes :

10 11 12 13 14 15

chain bonds :

1-2 1-5 5-6 6-7 7-12 16-17 17-18 17-19

ring bonds :

10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds :

1-2 1-5 7-12 17-19

exact bonds :

5-6 6-7 16-17 17-18

normalized bonds :

10-11 10-15 11-12 12-13 13-14 14-15

isolated ring systems :

containing 10 :

Connectivity :

2:1 E exact RC ring/chain

Match level :

1:Atom 2:CLASS 5:CLASS 6:CLASS 7:CLASS 10:Atom 11:Atom 12:Atom
13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS

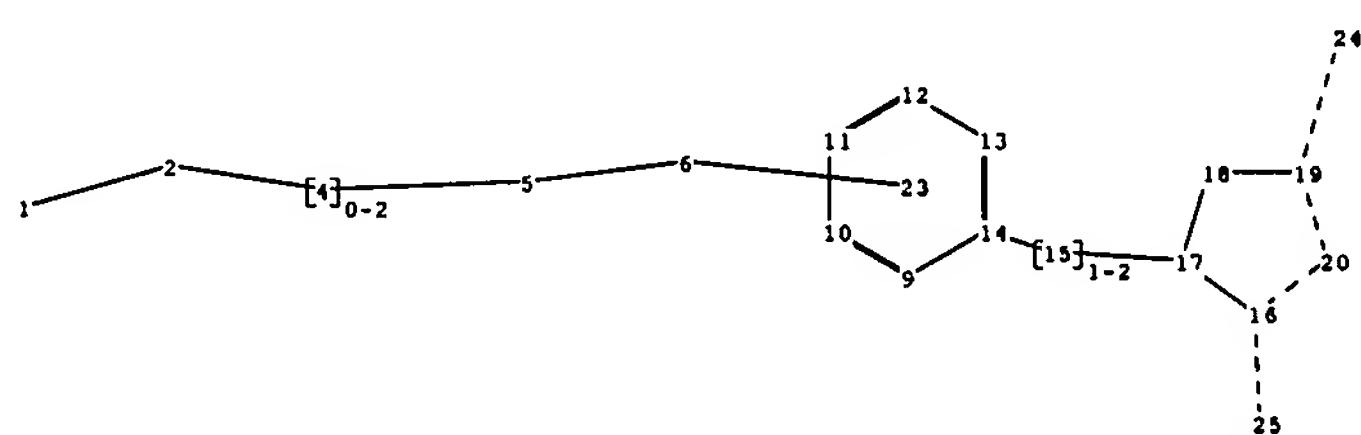
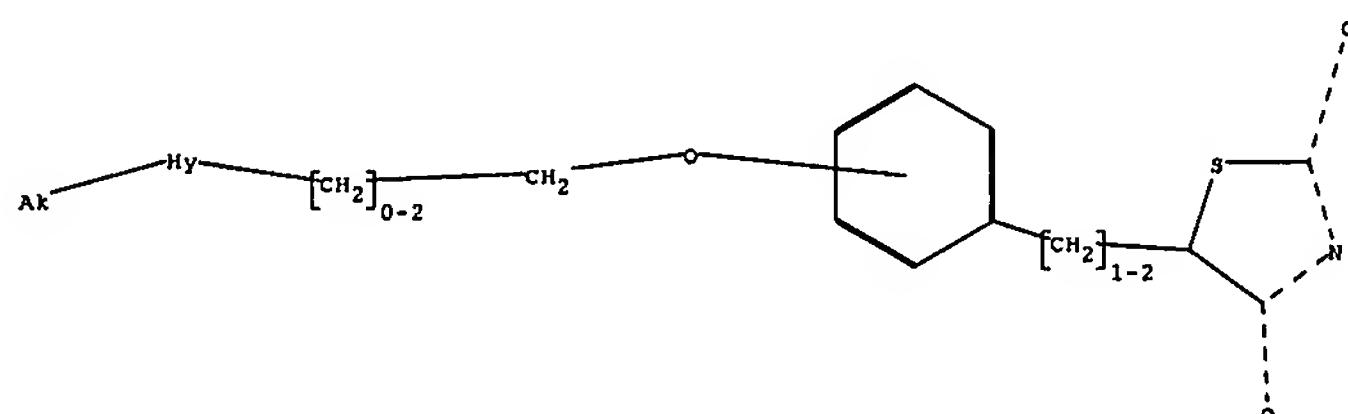
Generic attributes :

1:

Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic

Element Count :

Node 1: Limited
N, N1
C, C5



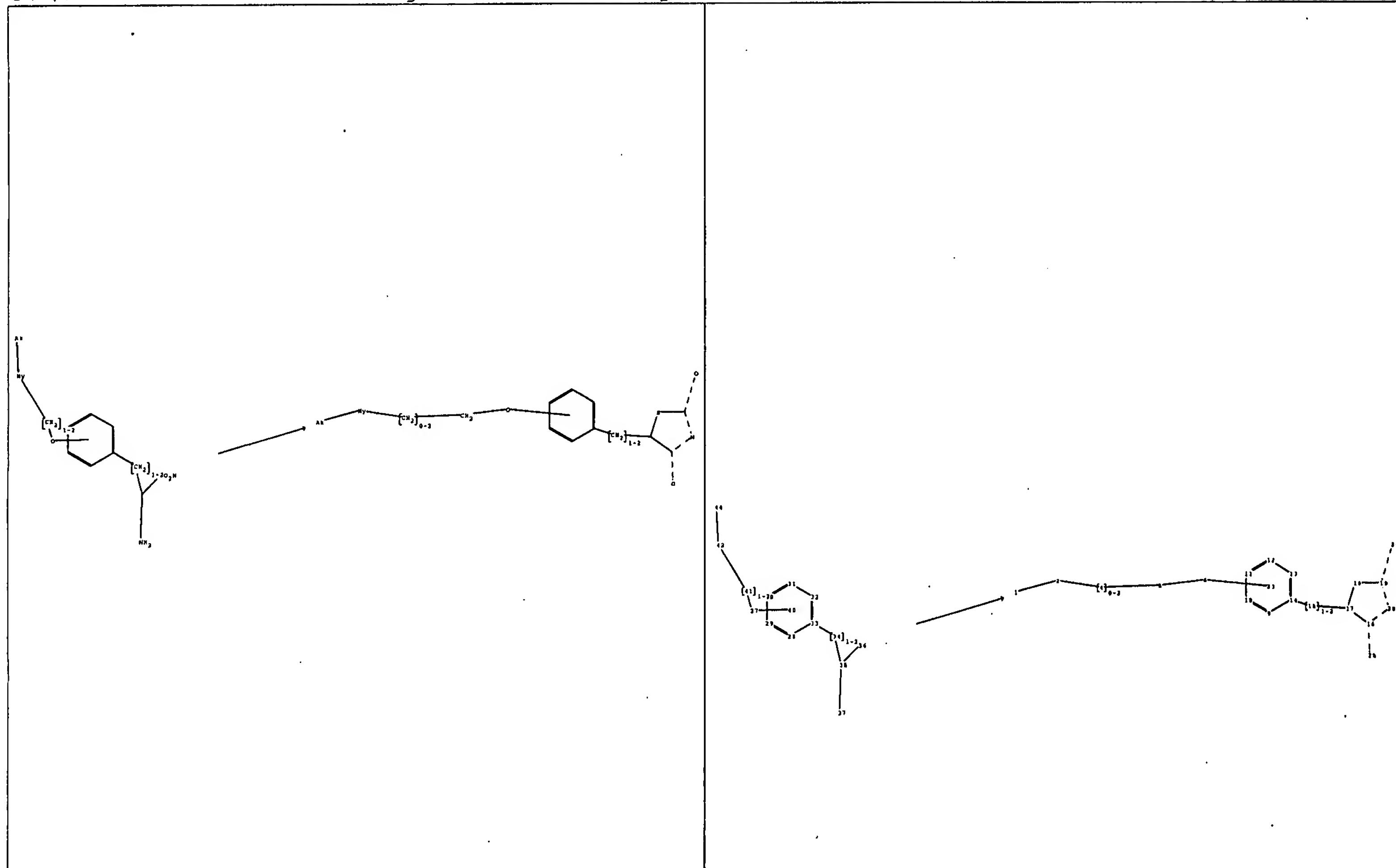
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chain nodes :
 1 2 4 5 6 15 24 25
ring nodes :
 9 10 11 12 13 14 16 17 18 19 20
chain bonds :
 1-2 2-4 4-5 5-6 14-15 15-17 16-25 19-24
ring bonds :
 9-10 9-14 10-11 11-12 12-13 13-14 16-17 16-20 17-18 18-19 19-20
exact/norm bonds :
 1-2 2-4 16-20 16-25 19-20 19-24
exact bonds :
 4-5 5-6 14-15 15-17 16-17 17-18 18-19
normalized bonds :
 9-10 9-14 10-11 11-12 12-13 13-14
isolated ring systems :
  containing 16 :
  / 

Match level :
 1:CLASS 2:Atom 4:CLASS 5:CLASS 6:CLASS 9:Atom 10:Atom 11:Atom
 12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom
 20:Atom 23:Atom 24:CLASS 25:CLASS
Generic attributes :
 2:
  Saturation : Unsaturated
  Number of Carbon Atoms : less than 7
  Number of Hetero Atoms : Exactly 1
  Type of Ring System : Monocyclic

Element Count :
  Node 2: Limited
  N, N1
  C, C5

```



chain nodes :

1 2 4 5 6 15 24 25 27 34 35 36 37 41 42 44

ring nodes :

9 10 11 12 13 14 16 17 18 19 20 28 29 30 31 32 33

chain bonds :

1-2 2-4 4-5 5-6 14-15 15-17 16-25 19-24 27-41 33-34 34-35 35-36
35-37 41-42 42-44

ring bonds :

9-10 9-14 10-11 11-12 12-13 13-14 16-17 16-20 17-18 18-19 19-20
28-29 28-33 29-30 30-31 31-32 32-33

exact/norm bonds :

1-2 2-4 16-20 16-25 19-20 19-24 35-37 41-42 42-44

exact bonds :

4-5 5-6 14-15 15-17 16-17 17-18 18-19 27-41 33-34 34-35 35-36

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14 28-29 28-33 29-30 30-31 31-32
32-33

isolated ring systems :

containing 16 : 28 :

Connectivity :

44:1 E exact RC ring/chain

Match level :

1:CLASS 2:Atom 4:CLASS 5:CLASS 6:CLASS 9:Atom 10:Atom 11:Atom
12:Atom 13:Atom 14:Atom 15:CLASS 16:Atom 17:Atom 18:Atom 19:Atom
20:Atom 23:Atom 24:CLASS 25:CLASS 27:CLASS 28:Atom 29:Atom 30:Atom
31:Atom 32:Atom 33:Atom 34:CLASS 35:CLASS 36:CLASS 37:CLASS 40:Atom
41:CLASS 42:Atom 44:CLASS

Generic attributes :

2:

Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1

Type of Ring System : Monocyclic
42:
Saturation : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic

fragments assigned reactant role:

containing 27

fragments assigned product role:

containing 1

Element Count :

Node 2: Limited

N, N1

C, C5

Node 42: Limited

C, C5

N, N1